



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 01:46 PM UTC

PDB ID : 1MLB / pdb_00001mlb
Title : MONOCLONAL ANTIBODY FAB D44.1 RAISED AGAINST CHICKEN EGG-WHITE LYSOZYME
Authors : Braden, B.C.; Souchon, H.; Eisele, J.-L.; Bentley, G.A.; Bhat, T.N.; Navaza, J.; Poljak, R.J.
Deposited on : 1995-03-08
Resolution : 2.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

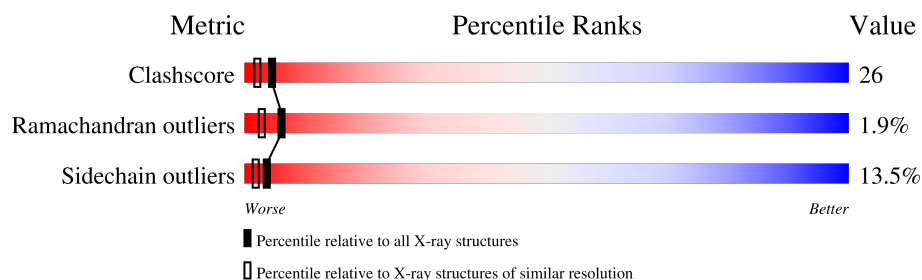
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	214	45% 41% 13% .
2	B	218	43% 34% 21% .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3424 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called IGG1-KAPPA D44.1 FAB (LIGHT CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	214	Total	C	N	O	S	0	2	0
			1670	1029	289	345	7			

- Molecule 2 is a protein called IGG1-KAPPA D44.1 FAB (HEAVY CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	218	Total	C	N	O	S	0	2	0
			1639	1033	269	329	8			

There are 17 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	5	GLN	VAL	conflict	PIR PC4202
B	11	VAL	LEU	conflict	PIR PC4202
B	26	GLY	ASP	conflict	PIR PC4202
B	28	THR	ARG	conflict	PIR PC4202
B	31	THR	SER	conflict	PIR PC4202
B	50	GLU	ASP	conflict	PIR PC4202
B	57	SER	ASN	conflict	PIR PC4202
B	59	TYR	ASN	conflict	PIR PC4202
B	63	LYS	ARG	conflict	PIR PC4202
B	98	ARG	ILE	conflict	PIR PC4202
B	99	GLY	PRO	conflict	PIR PC4202
B	101	GLY	-	insertion	PIR PC4202
B	102	ASN	-	insertion	PIR PC4202
B	103	TYR	-	insertion	PIR PC4202
B	104	GLY	-	insertion	PIR PC4202
B	118	SER	LYS	conflict	PIR PC4202
B	125	PHE	TYR	conflict	PIR PC4202

- Molecule 3 is water.

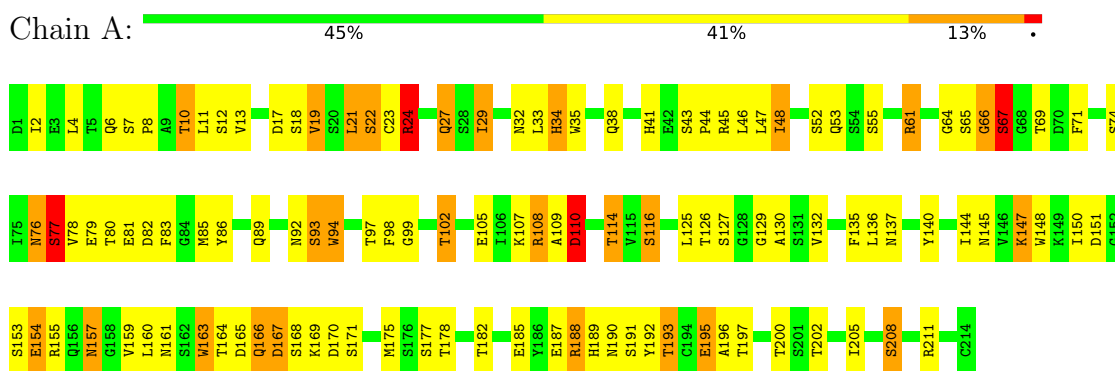
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	71	Total 71	O 71	0	0
3	B	44	Total 44	O 44	0	0

3 Residue-property plots [i](#)

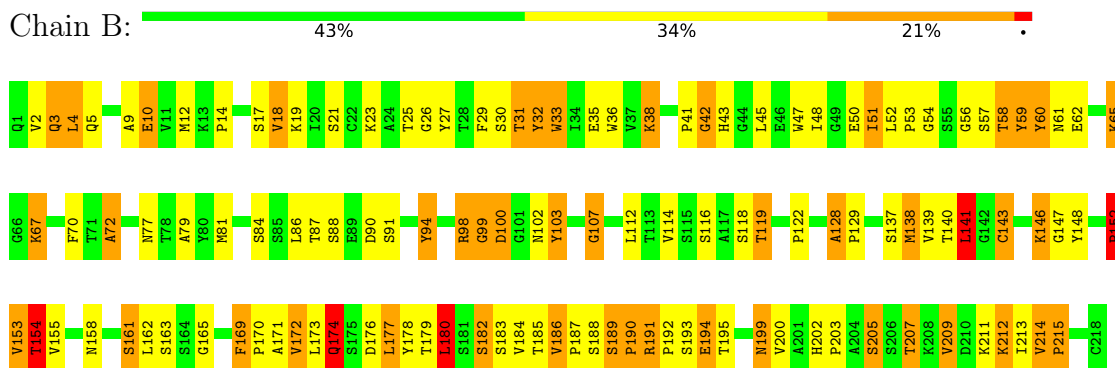
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

- Molecule 1: IGG1-KAPPA D44.1 FAB (LIGHT CHAIN)



- Molecule 2: IGG1-KAPPA D44.1 FAB (HEAVY CHAIN)



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	79.70Å 136.20Å 43.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	7.00 – 2.10	Depositor
% Data completeness (in resolution range)	(Not available) (7.00-2.10)	Depositor
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.181 , 0.274	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3424	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.25	3/1717 (0.2%)	2.27	79/2326 (3.4%)
2	B	1.26	0/1695	2.18	77/2315 (3.3%)
All	All	1.26	3/3412 (0.1%)	2.22	156/4641 (3.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	129	GLY	N-CA	7.26	1.52	1.44
1	A	55	SER	C-N	-5.41	1.26	1.33
1	A	53	GLN	N-CA	5.36	1.52	1.45

All (156) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	108	ARG	NE-CZ-NH1	10.37	131.87	121.50
1	A	102	THR	CA-C-O	-9.65	110.01	120.24
1	A	41	HIS	CA-CB-CG	-9.39	104.41	113.80
2	B	100	ASP	CA-CB-CG	8.94	121.54	112.60
2	B	88	SER	O-C-N	8.85	133.16	122.27
2	B	114	VAL	CA-C-O	-8.63	111.18	120.59
1	A	211	ARG	NE-CZ-NH2	-8.54	111.51	119.20
2	B	18	VAL	O-C-N	8.40	131.99	123.00
1	A	80	THR	N-CA-CB	8.28	122.41	110.16
1	A	102	THR	O-C-N	8.22	132.89	123.27
1	A	187	GLU	CB-CG-CD	7.80	125.86	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	18	SER	CA-C-O	-7.75	111.80	120.32
1	A	167	ASP	CA-CB-CG	-7.63	104.97	112.60
2	B	59	TYR	CA-C-O	7.52	128.63	120.43
1	A	99	GLY	CA-C-N	7.45	128.25	119.98
1	A	99	GLY	C-N-CA	7.45	128.25	119.98
1	A	10	THR	CA-CB-OG1	-7.42	98.47	109.60
2	B	12	MET	O-C-N	7.39	132.76	123.15
2	B	152	PRO	N-CA-CB	-7.36	94.51	102.60
2	B	189	SER	O-C-N	7.34	126.18	120.38
2	B	193	SER	CA-C-O	7.34	127.85	119.27
2	B	176	ASP	CA-CB-CG	-7.31	105.29	112.60
2	B	21	SER	CA-C-O	7.22	129.80	121.28
1	A	144	ILE	O-C-N	7.14	131.50	122.57
1	A	190	ASN	OD1-CG-ND2	7.07	129.67	122.60
1	A	85	MET	N-CA-CB	-7.01	98.96	110.52
1	A	211	ARG	NE-CZ-NH1	6.99	128.49	121.50
1	A	38	GLN	CG-CD-NE2	-6.92	106.02	116.40
2	B	60	TYR	O-C-N	6.83	132.07	123.19
1	A	166	GLN	OE1-CD-NE2	6.81	129.41	122.60
1	A	110	ASP	CA-CB-CG	-6.80	105.80	112.60
2	B	177	LEU	CB-CA-C	6.69	121.75	109.71
1	A	32	ASN	OD1-CG-ND2	6.67	129.27	122.60
2	B	119	THR	CB-CA-C	6.64	117.96	109.80
1	A	45	ARG	CA-CB-CG	6.57	127.25	114.10
2	B	5	GLN	OE1-CD-NE2	6.57	129.17	122.60
1	A	74	SER	CA-C-O	-6.55	113.62	120.70
2	B	143	CYS	CA-C-O	-6.54	113.06	120.32
1	A	77	SER	O-C-N	6.50	131.23	122.59
1	A	10	THR	O-C-N	6.46	130.76	123.27
2	B	143	CYS	O-C-N	6.45	130.85	123.31
2	B	107	GLY	N-CA-C	-6.44	102.47	112.85
1	A	193	THR	O-C-N	6.42	131.10	123.27
1	A	76	ASN	O-C-N	6.42	130.83	122.68
1	A	94	TRP	CB-CA-C	6.40	117.58	108.68
1	A	79	GLU	CA-C-O	-6.38	113.58	121.88
2	B	23	LYS	CA-C-O	-6.35	113.81	121.05
1	A	168	SER	N-CA-C	6.33	118.26	111.36
2	B	114	VAL	O-C-N	6.30	131.29	122.97
2	B	72	ALA	CA-C-O	-6.27	113.99	120.89
2	B	19	LYS	CA-C-N	6.26	131.26	123.12
2	B	19	LYS	C-N-CA	6.26	131.26	123.12
2	B	86	LEU	CB-CA-C	6.23	120.06	109.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	97	THR	O-C-N	6.22	130.36	123.33
1	A	107	LYS	CA-C-N	6.22	134.07	123.01
1	A	107	LYS	C-N-CA	6.22	134.07	123.01
2	B	141	LEU	N-CA-CB	-6.19	101.32	110.85
2	B	61	ASN	OD1-CG-ND2	6.09	128.69	122.60
2	B	79	ALA	CB-CA-C	6.04	119.77	109.80
2	B	141	LEU	CB-CA-C	6.03	120.57	109.71
2	B	199	ASN	CA-CB-CG	6.02	118.62	112.60
1	A	116	SER	CA-C-O	-6.00	113.76	120.66
2	B	171	ALA	CA-C-O	-5.99	115.03	121.56
1	A	137	ASN	CA-C-N	5.98	132.96	121.54
1	A	137	ASN	C-N-CA	5.98	132.96	121.54
1	A	129	GLY	N-CA-C	-5.96	102.01	111.18
1	A	48	ILE	CB-CG1-CD1	5.95	126.29	113.80
1	A	195	GLU	O-C-N	-5.92	116.40	123.27
1	A	44	PRO	CB-CA-C	5.91	118.80	111.23
1	A	108	ARG	NE-CZ-NH2	-5.90	113.89	119.20
1	A	193	THR	CA-CB-OG1	-5.84	100.83	109.60
1	A	27	GLN	O-C-N	5.81	130.32	122.59
2	B	33	TRP	O-C-N	5.80	130.07	122.93
2	B	169	PHE	CB-CA-C	5.78	117.18	108.86
2	B	54	GLY	CA-C-N	5.78	128.28	120.65
2	B	54	GLY	C-N-CA	5.78	128.28	120.65
2	B	103	TYR	CA-C-O	-5.77	113.97	120.32
1	A	105	GLU	CB-CG-CD	5.77	122.40	112.60
2	B	138	MET	CA-C-O	-5.76	115.15	121.89
2	B	209	VAL	CB-CA-C	5.74	119.39	110.83
1	A	129	GLY	CA-C-O	-5.73	115.86	121.76
1	A	44	PRO	CA-C-O	5.72	128.19	121.56
2	B	119	THR	CA-CB-OG1	-5.72	101.03	109.60
2	B	186	VAL	N-CA-C	5.70	113.87	109.19
1	A	107	LYS	CA-C-O	5.70	127.19	120.69
1	A	98	PHE	CA-CB-CG	5.69	119.49	113.80
2	B	32	TYR	N-CA-C	5.69	119.34	110.17
1	A	163	TRP	CA-C-O	-5.65	114.59	120.70
1	A	66	GLY	CA-C-O	-5.64	117.53	122.16
1	A	148	TRP	CA-C-N	-5.63	113.60	122.73
1	A	148	TRP	C-N-CA	-5.63	113.60	122.73
1	A	79	GLU	CG-CD-OE1	5.63	131.35	118.40
1	A	154	GLU	CB-CG-CD	5.63	122.17	112.60
2	B	209	VAL	CA-C-O	5.62	126.43	120.48
2	B	58	THR	CA-CB-OG1	-5.61	101.19	109.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	174	GLN	CB-CA-C	5.60	118.76	111.42
1	A	18	SER	O-C-N	5.56	129.83	123.27
2	B	162	LEU	CA-C-O	-5.54	114.65	121.02
1	A	140	TYR	CB-CA-C	5.52	116.82	109.65
1	A	89	GLN	CG-CD-OE1	5.51	131.83	120.80
2	B	45	LEU	N-CA-CB	-5.51	101.26	110.80
2	B	128	ALA	O-C-N	5.50	128.80	121.70
1	A	83	PHE	CA-CB-CG	5.49	119.29	113.80
2	B	94	TYR	O-C-N	5.46	130.32	123.23
2	B	138	MET	N-CA-C	-5.45	102.68	110.59
1	A	107	LYS	O-C-N	-5.45	116.66	123.04
2	B	184	VAL	CA-C-O	-5.44	114.52	120.72
1	A	126	THR	CA-CB-OG1	-5.41	101.48	109.60
2	B	98	ARG	NH1-CZ-NH2	5.41	126.33	119.30
1	A	74	SER	O-C-N	5.40	130.25	123.23
2	B	10	GLU	CA-CB-CG	5.38	124.87	114.10
1	A	64	GLY	N-CA-C	-5.37	102.96	110.96
2	B	56	GLY	N-CA-C	-5.35	107.41	114.95
2	B	209	VAL	O-C-N	-5.35	117.56	123.18
1	A	92	ASN	CA-CB-CG	-5.34	107.26	112.60
1	A	64	GLY	O-C-N	5.34	128.53	123.57
1	A	61	ARG	CA-C-N	5.34	129.13	121.50
1	A	61	ARG	C-N-CA	5.34	129.13	121.50
2	B	12	MET	CA-C-O	-5.34	115.20	121.44
2	B	161	SER	CA-C-O	-5.34	115.40	120.90
2	B	14	PRO	CB-CA-C	5.31	118.27	111.21
2	B	153	VAL	N-CA-C	-5.30	100.99	109.20
2	B	12	MET	CG-SD-CE	5.29	112.55	100.90
1	A	52	SER	CA-C-N	-5.29	111.43	122.07
1	A	52	SER	C-N-CA	-5.29	111.43	122.07
1	A	108	ARG	CB-CA-C	-5.29	100.01	111.11
2	B	147	GLY	O-C-N	-5.26	115.86	122.70
1	A	61	ARG	NH1-CZ-NH2	-5.23	112.50	119.30
1	A	24[A]	ARG	CA-C-O	-5.23	115.23	121.56
1	A	24[B]	ARG	CA-C-O	-5.23	115.23	121.56
2	B	165	GLY	CA-C-N	5.22	128.87	121.66
2	B	165	GLY	C-N-CA	5.22	128.87	121.66
1	A	86	TYR	O-C-N	5.21	130.00	123.12
1	A	29	ILE	O-C-N	5.18	127.74	122.09
1	A	93	SER	O-C-N	5.18	129.05	123.10
2	B	179	THR	CA-C-N	5.15	130.55	122.21
2	B	179	THR	C-N-CA	5.15	130.55	122.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	9	ALA	CA-C-O	-5.15	116.09	121.55
2	B	154	THR	CA-CB-OG1	-5.14	101.89	109.60
2	B	50	GLU	CG-CD-OE2	5.13	130.21	118.40
2	B	140	THR	O-C-N	5.13	129.33	123.27
2	B	65	LYS	CA-C-O	-5.13	113.18	120.51
2	B	214	VAL	O-C-N	5.12	126.94	121.10
2	B	99	GLY	CA-C-O	-5.11	116.94	121.64
1	A	127	SER	N-CA-C	-5.08	106.91	113.01
2	B	31	THR	CA-CB-OG1	-5.08	101.98	109.60
2	B	180	LEU	N-CA-CB	-5.08	102.85	111.69
2	B	158	ASN	CA-CB-CG	5.07	117.67	112.60
2	B	38	LYS	CB-CA-C	-5.06	100.96	109.72
2	B	62	GLU	CA-CB-CG	5.06	124.21	114.10
1	A	65	SER	CA-C-O	-5.05	115.91	121.31
2	B	182	SER	CB-CA-C	5.04	119.33	109.35
1	A	53	GLN	CA-C-O	-5.03	115.79	121.72
1	A	105	GLU	CA-C-N	5.01	128.70	121.18
1	A	105	GLU	C-N-CA	5.01	128.70	121.18
2	B	36	TRP	O-C-N	5.01	129.17	123.31

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	188[A]	ARG	Sidechain
1	A	188[B]	ARG	Sidechain
1	A	24[A]	ARG	Sidechain
1	A	24[B]	ARG	Sidechain

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1670	0	1590	74	0
2	B	1639	0	1582	102	0
3	A	71	0	0	0	0
3	B	44	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	3424	0	3172	167	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 26.

All (167) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:188[B]:ARG:CZ	1:A:188[B]:ARG:NE	1.82	1.42
1:A:24[B]:ARG:CG	1:A:24[B]:ARG:CD	2.02	1.38
2:B:48:ILE:HD13	2:B:81[A]:MET:HE1	1.33	1.10
2:B:51:ILE:HG13	2:B:58:THR:HG22	1.45	0.97
2:B:187:PRO:O	2:B:190:PRO:HD2	1.73	0.89
2:B:48:ILE:HG21	2:B:81[A]:MET:CE	2.02	0.89
2:B:173:LEU:HD13	2:B:178:TYR:CE1	2.09	0.88
2:B:212:LYS:HB2	2:B:212:LYS:NZ	1.91	0.85
2:B:35:GLU:HG3	2:B:103:TYR:CE1	2.12	0.83
2:B:189:SER:HB2	2:B:190:PRO:HD3	1.60	0.82
1:A:160:LEU:HD23	2:B:172:VAL:HG21	1.62	0.81
1:A:61:ARG:NH1	1:A:82:ASP:OD1	2.16	0.79
1:A:188[B]:ARG:NE	1:A:188[B]:ARG:NH2	2.30	0.78
1:A:160:LEU:HD23	2:B:172:VAL:CG2	2.13	0.77
1:A:147:LYS:HB2	1:A:147:LYS:HZ3	1.50	0.76
2:B:48:ILE:HG21	2:B:81[A]:MET:HE1	1.66	0.76
2:B:187:PRO:HG2	2:B:190:PRO:HG2	1.67	0.76
2:B:141:LEU:HD11	2:B:191[B]:ARG:NE	2.02	0.75
2:B:3:GLN:HE21	2:B:3:GLN:HA	1.51	0.74
1:A:155:ARG:NE	1:A:157:ASN:HD22	1.87	0.72
2:B:47:TRP:HH2	2:B:59:TYR:HD2	1.36	0.72
1:A:2:ILE:HD13	1:A:29:ILE:HG22	1.71	0.72
2:B:212:LYS:NZ	2:B:212:LYS:CB	2.53	0.72
1:A:61:ARG:HH11	1:A:82:ASP:CG	1.98	0.72
2:B:190:PRO:HA	2:B:194:GLU:HG2	1.71	0.71
2:B:3:GLN:HE21	2:B:3:GLN:CA	2.03	0.71
2:B:48:ILE:CD1	2:B:81[A]:MET:HE1	2.18	0.70
1:A:76:ASN:O	1:A:77:SER:HB2	1.90	0.70
1:A:29:ILE:HD11	1:A:33:LEU:HB2	1.74	0.69
1:A:155:ARG:HE	1:A:157:ASN:HD22	1.39	0.69
2:B:138:MET:HE3	2:B:185:THR:HG22	1.74	0.69
2:B:141:LEU:HD11	2:B:191[B]:ARG:CD	2.23	0.69
2:B:47:TRP:HH2	2:B:59:TYR:CD2	2.10	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:19:VAL:HG23	1:A:21:LEU:CD1	2.23	0.68
1:A:155:ARG:NE	1:A:157:ASN:ND2	2.42	0.68
1:A:193:THR:OG1	1:A:208:SER:HB3	1.94	0.67
2:B:173:LEU:HD13	2:B:178:TYR:CD1	2.30	0.66
2:B:203:PRO:HD2	3:B:454:HOH:O	1.94	0.66
2:B:205:SER:HB2	2:B:207:THR:OG1	1.95	0.66
1:A:29:ILE:CD1	1:A:33:LEU:HB2	2.27	0.65
2:B:139:VAL:N	2:B:186:VAL:O	2.31	0.64
1:A:19:VAL:HG13	1:A:78:VAL:HG21	1.78	0.64
1:A:61:ARG:NH1	1:A:82:ASP:CG	2.54	0.64
1:A:108:ARG:HD2	1:A:170:ASP:O	1.98	0.63
1:A:19:VAL:HG13	1:A:78:VAL:CG2	2.29	0.62
2:B:202:HIS:ND1	2:B:205:SER:OG	2.28	0.61
2:B:212:LYS:HB2	2:B:212:LYS:HZ2	1.64	0.61
2:B:52:LEU:HD12	2:B:53:PRO:HD2	1.83	0.61
1:A:151:ASP:OD2	1:A:189:HIS:HB3	2.00	0.60
2:B:51:ILE:HG13	2:B:58:THR:CG2	2.26	0.60
2:B:137:SER:O	2:B:188:SER:OG	2.19	0.59
2:B:138:MET:HB3	2:B:185:THR:CG2	2.33	0.59
1:A:47:LEU:O	1:A:48:ILE:HD13	2.02	0.59
1:A:188[B]:ARG:NE	1:A:188[B]:ARG:NH1	2.37	0.59
2:B:141:LEU:HD21	2:B:191[B]:ARG:HG3	1.84	0.59
2:B:4:LEU:O	2:B:107:GLY:HA2	2.03	0.58
1:A:94:TRP:HB3	2:B:59:TYR:CZ	2.37	0.58
1:A:24[B]:ARG:CD	1:A:24[B]:ARG:NE	2.66	0.58
2:B:173:LEU:HD12	2:B:177:LEU:O	2.03	0.58
2:B:47:TRP:CH2	2:B:59:TYR:CD2	2.92	0.57
1:A:19:VAL:HG23	1:A:21:LEU:HD12	1.87	0.57
2:B:191[B]:ARG:CD	2:B:191[B]:ARG:HB3	2.32	0.57
1:A:94:TRP:HB3	2:B:59:TYR:CE2	2.41	0.56
1:A:136:LEU:HD21	1:A:196:ALA:HB2	1.87	0.56
1:A:61:ARG:NH1	1:A:82:ASP:OD2	2.33	0.56
1:A:8:PRO:O	1:A:102:THR:HG23	2.06	0.56
2:B:67:LYS:NZ	2:B:90:ASP:OD2	2.38	0.56
2:B:187:PRO:HG2	2:B:190:PRO:CG	2.35	0.55
2:B:47:TRP:CH2	2:B:59:TYR:HD2	2.23	0.55
1:A:33:LEU:HD13	1:A:71:PHE:CD2	2.43	0.54
1:A:108:ARG:HG3	1:A:171:SER:HB2	1.90	0.54
2:B:212:LYS:HB2	2:B:212:LYS:HZ3	1.71	0.54
1:A:182:THR:OG1	1:A:185:GLU:HB2	2.08	0.53
2:B:129:PRO:HD3	2:B:141:LEU:HD12	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3:GLN:HA	2:B:3:GLN:NE2	2.24	0.52
1:A:147:LYS:HB2	1:A:147:LYS:NZ	2.20	0.52
1:A:66:GLY:O	1:A:67:SER:HB2	2.09	0.52
2:B:33:TRP:O	2:B:99:GLY:N	2.36	0.52
2:B:67:LYS:HE2	2:B:84:SER:O	2.10	0.51
2:B:122:PRO:HB3	2:B:148:TYR:HB3	1.93	0.51
1:A:17:ASP:O	1:A:78:VAL:N	2.33	0.51
1:A:6:GLN:HA	1:A:22:SER:O	2.11	0.51
2:B:118:SER:O	2:B:119:THR:C	2.50	0.51
1:A:19:VAL:CG1	1:A:78:VAL:HG21	2.41	0.50
2:B:2:VAL:HG13	2:B:27:TYR:CD1	2.46	0.50
2:B:199:ASN:HA	2:B:209:VAL:O	2.11	0.50
2:B:29:PHE:O	2:B:53:PRO:HG2	2.12	0.50
1:A:24[A]:ARG:HH21	1:A:69:THR:HB	1.77	0.50
2:B:141:LEU:HD11	2:B:191[B]:ARG:HD2	1.92	0.50
2:B:91:SER:HA	2:B:112:LEU:O	2.12	0.50
1:A:2:ILE:HD13	1:A:29:ILE:CG2	2.41	0.49
1:A:34:HIS:ND1	2:B:102:ASN:HB3	2.27	0.49
2:B:47:TRP:CZ3	2:B:59:TYR:HE2	2.30	0.49
1:A:192:TYR:O	1:A:208:SER:CB	2.61	0.49
2:B:67:LYS:O	2:B:67:LYS:HG3	2.12	0.49
2:B:137:SER:C	2:B:188:SER:HG	2.19	0.49
2:B:51:ILE:HD13	2:B:72:ALA:HB2	1.94	0.48
2:B:32:TYR:N	2:B:32:TYR:CD1	2.82	0.48
1:A:23:CYS:HB2	1:A:35:TRP:CH2	2.49	0.47
1:A:19:VAL:CG2	1:A:21:LEU:HD11	2.45	0.47
1:A:175:MET:HE3	1:A:175:MET:HB2	1.57	0.46
2:B:47:TRP:HZ3	2:B:59:TYR:HE2	1.64	0.46
2:B:152:PRO:O	2:B:152:PRO:HG2	2.16	0.46
1:A:147:LYS:NZ	1:A:154:GLU:OE2	2.44	0.46
1:A:10:THR:HG22	1:A:11:LEU:N	2.31	0.46
1:A:195:GLU:HA	1:A:205:ILE:O	2.17	0.45
2:B:47:TRP:CZ3	2:B:59:TYR:CE2	3.04	0.45
1:A:110:ASP:HB3	1:A:200:THR:HG22	1.97	0.45
2:B:173:LEU:HD12	2:B:173:LEU:HA	1.90	0.45
2:B:60:TYR:CE1	2:B:70:PHE:CD2	3.05	0.45
2:B:190:PRO:HA	2:B:194:GLU:CG	2.43	0.45
1:A:163:TRP:O	2:B:170:PRO:HG2	2.17	0.45
2:B:25:THR:HG22	2:B:26:GLY:N	2.31	0.45
2:B:189:SER:HB2	2:B:190:PRO:CD	2.39	0.45
1:A:165:ASP:O	1:A:166:GLN:C	2.60	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:212:LYS:HE2	2:B:212:LYS:HB3	1.66	0.45
2:B:128:ALA:HB1	2:B:129:PRO:HD2	1.98	0.44
1:A:125:LEU:CD1	1:A:130:ALA:HB2	2.48	0.44
2:B:141:LEU:CD1	2:B:191[B]:ARG:HD2	2.47	0.44
1:A:164:THR:HG23	2:B:169:PHE:CD1	2.53	0.44
2:B:31:THR:HG22	2:B:32:TYR:CE1	2.52	0.44
1:A:167:ASP:OD1	1:A:167:ASP:C	2.61	0.44
1:A:188[B]:ARG:NE	1:A:188[B]:ARG:HH21	2.12	0.44
2:B:38:LYS:HG3	2:B:94:TYR:CE1	2.53	0.44
1:A:145:ASN:HD22	1:A:145:ASN:HA	1.50	0.43
2:B:42:GLY:O	2:B:43:HIS:CG	2.71	0.43
1:A:159:VAL:HA	1:A:178:THR:O	2.18	0.43
2:B:48:ILE:HG21	2:B:81[A]:MET:HE3	1.93	0.43
1:A:169:LYS:HA	1:A:169:LYS:HD3	1.48	0.43
2:B:38:LYS:HB2	2:B:48:ILE:HD11	2.01	0.43
1:A:192:TYR:O	1:A:208:SER:HB3	2.19	0.43
2:B:187:PRO:C	2:B:189:SER:H	2.27	0.43
2:B:3:GLN:O	2:B:4:LEU:HD23	2.18	0.43
2:B:27:TYR:CE2	2:B:98:ARG:HD2	2.54	0.43
1:A:114:THR:O	1:A:114:THR:HG22	2.18	0.42
2:B:194:GLU:OE1	2:B:194:GLU:HA	2.19	0.42
1:A:125:LEU:HD12	1:A:125:LEU:HA	1.76	0.42
2:B:191[A]:ARG:HH11	2:B:215:PRO:HD3	1.85	0.42
2:B:155:VAL:HG21	2:B:180:LEU:HD21	2.02	0.42
1:A:67:SER:HA	1:A:71:PHE:HE1	1.84	0.42
1:A:13:VAL:HG21	1:A:19:VAL:HG11	2.02	0.42
1:A:109:ALA:O	1:A:110:ASP:C	2.63	0.42
1:A:135:PHE:CE2	2:B:183:SER:HB3	2.54	0.42
2:B:29:PHE:HB3	2:B:77:ASN:ND2	2.35	0.42
2:B:60:TYR:CE1	2:B:70:PHE:CE2	3.07	0.42
1:A:150:ILE:O	1:A:151:ASP:C	2.63	0.41
2:B:10:GLU:HG3	2:B:18:VAL:HG21	2.01	0.41
2:B:187:PRO:HG2	2:B:190:PRO:CD	2.49	0.41
2:B:154:THR:O	2:B:200:VAL:HA	2.20	0.41
2:B:191[A]:ARG:NH1	2:B:215:PRO:HG3	2.35	0.41
2:B:128:ALA:HB2	2:B:213:ILE:HG22	2.01	0.41
1:A:34:HIS:CG	2:B:102:ASN:HB3	2.56	0.41
1:A:161:ASN:ND2	1:A:177:SER:OG	2.53	0.41
2:B:25:THR:CG2	2:B:26:GLY:N	2.83	0.41
1:A:13:VAL:HG11	1:A:78:VAL:HG21	2.03	0.41
2:B:153:VAL:HG12	2:B:202:HIS:CD2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:192:PRO:HB3	2:B:215:PRO:HG3	2.03	0.41
1:A:34:HIS:CD2	1:A:34:HIS:N	2.88	0.40
2:B:146:LYS:HE2	2:B:174:GLN:OE1	2.21	0.40
2:B:211:LYS:HD3	2:B:211:LYS:HA	1.81	0.40
1:A:2:ILE:HG12	1:A:27:GLN:CG	2.51	0.40
2:B:187:PRO:C	2:B:189:SER:N	2.78	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	214/214 (100%)	201 (94%)	10 (5%)	3 (1%)	9	5
2	B	218/218 (100%)	201 (92%)	12 (6%)	5 (2%)	5	2
All	All	432/432 (100%)	402 (93%)	22 (5%)	8 (2%)	6	3

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	67	SER
1	A	110	ASP
2	B	190	PRO
2	B	42	GLY
1	A	77	SER
2	B	100	ASP
2	B	65	LYS
2	B	41	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	196/194 (101%)	173 (88%)	23 (12%)	5	3
2	B	186/184 (101%)	157 (84%)	29 (16%)	2	1
All	All	382/378 (101%)	330 (86%)	52 (14%)	4	2

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LEU
1	A	7	SER
1	A	12	SER
1	A	19	VAL
1	A	21	LEU
1	A	22	SER
1	A	34	HIS
1	A	43	SER
1	A	46	LEU
1	A	67	SER
1	A	77	SER
1	A	81	GLU
1	A	93	SER
1	A	114	THR
1	A	116	SER
1	A	132	VAL
1	A	147	LYS
1	A	153	SER
1	A	157	ASN
1	A	191	SER
1	A	197	THR
1	A	202	THR
1	A	208	SER
2	B	3	GLN
2	B	4	LEU
2	B	17	SER
2	B	30	SER

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Mol	Chain	Res	Type
2	B	51	ILE
2	B	57	SER
2	B	67	LYS
2	B	87	THR
2	B	116	SER
2	B	141	LEU
2	B	143	CYS
2	B	146	LYS
2	B	152	PRO
2	B	154	THR
2	B	161	SER
2	B	163	SER
2	B	172	VAL
2	B	174	GLN
2	B	180	LEU
2	B	182	SER
2	B	191[A]	ARG
2	B	191[B]	ARG
2	B	194	GLU
2	B	195	THR
2	B	205	SER
2	B	207	THR
2	B	212	LYS
2	B	214	VAL
2	B	215	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	GLN
1	A	76	ASN
1	A	145	ASN
1	A	156	GLN
1	A	157	ASN
1	A	161	ASN
1	A	210	ASN
1	A	212	ASN
2	B	1	GLN
2	B	3	GLN
2	B	39	GLN
2	B	43	HIS
2	B	77	ASN

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Mol	Chain	Res	Type
2	B	82	GLN
2	B	102	ASN
2	B	167	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.